

Sharpening the Norm Bound in the Subspace Perturbation Theory*

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Abstract. Let A be a (possibly unbounded) self-adjoint operator on a separable Hilbert space \mathfrak{H} . Assume that σ is an isolated component of the spectrum of A , that is, $\text{dist}(\sigma, \Sigma) = d > 0$ where $\Sigma = \text{spec}(A) \setminus \sigma$. Suppose that V is a bounded self-adjoint operator on \mathfrak{H} such that $\|V\| < d/2$ and let $L = A + V$, $\text{Dom}(L) = \text{Dom}(A)$. Denote by P the spectral projection of A associated with the spectral set σ and let Q be the spectral projection of L corresponding to the closed $\|V\|$ -neighborhood of σ . Introducing the sequence

$$\varkappa_n = \frac{1}{2} \left(1 - \frac{(\pi^2 - 4)^n}{(\pi^2 + 4)^n} \right), \quad n \in \{0\} \cup \mathbb{N},$$

we prove that the following bound holds:

$$\arcsin(\|P - Q\|) \leq M_\star \left(\frac{\|V\|}{d} \right),$$

where the estimating function $M_\star(x)$, $x \in [0, \frac{1}{2})$, is given by

$$M_\star(x) = \frac{1}{2} n_\#(x) \arcsin \left(\frac{4\pi}{\pi^2 + 4} \right) + \frac{1}{2} \arcsin \left(\frac{\pi(x - \varkappa_{n_\#(x)}))}{1 - 2\varkappa_{n_\#(x)}} \right),$$

with $n_\#(x) = \max \{n \mid n \in \{0\} \cup \mathbb{N}, \varkappa_n \leq x\}$. The bound obtained is essentially stronger than the previously known estimates for $\|P - Q\|$. Furthermore, this bound ensures that $\|P - Q\| < 1$ and, thus, that the spectral subspaces $\text{Ran}(P)$ and $\text{Ran}(Q)$ are in the acute-angle case whenever $\|V\| < c_\star d$, where

$$c_\star = 16 \frac{\pi^6 - 2\pi^4 + 32\pi^2 - 32}{(\pi^2 + 4)^4} = 0.454169 \dots$$

Our proof of the above results is based on using the triangle inequality for the maximal angle between subspaces and on employing the a priori generic $\sin 2\theta$ estimate for the variation of a spectral subspace. As an example, the boundedly perturbed quantum harmonic oscillator is discussed.

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1. Introduction

One of fundamental problems of operator perturbation theory is to study variation of the spectral subspace corresponding to a subset of the spectrum of a closed linear operator that is subject to a perturbation. This is an especially important issue in perturbation theory of self-adjoint operators.

Assume that A is a self-adjoint operator on a separable Hilbert space \mathfrak{H} . It is well known (see, e.g., [13]) that if V is a bounded self-adjoint perturbation of A then the spectrum, $\text{spec}(L)$, of the perturbed operator $L = A + V$, $\text{Dom}(L) = \text{Dom}(A)$, lies in the closed $\|V\|$ -neighborhood $\mathcal{O}_{\|V\|}(\text{spec}(A))$ of the spectrum of A . Hence, if the spectrum of A has an isolated component σ separated from its complement $\Sigma = \text{spec}(A) \setminus \sigma$ by gaps of length greater than or equal to $d > 0$, that is, if

$$\text{dist}(\sigma, \Sigma) = d > 0, \quad (1.1)$$

then the spectrum of L will also consist of two disjoint components, $\omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\sigma)$ and $\Omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\Sigma)$, provided that

$$\|V\| < d/2. \quad (1.2)$$

Under condition (1.2) one may think of the separated spectral components ω and Ω of the perturbed operator L as the result of the perturbation of the initial disjoint spectral sets σ and Σ , respectively. Clearly, this condition is sharp in the sense that if $\|V\| > d/2$, the perturbed operator L may not have separated parts of the spectrum at all.

Assuming (1.2), let $P = E_A(\sigma)$ and $Q = E_L(\omega)$ be the spectral projections of the (self-adjoint) operators A and L associated with the unperturbed and perturbed isolated spectral sets σ and ω , respectively. A still unsolved problem is to answer the following fundamental question:

- (i) *Is it true that under the single spectral condition (1.1) the perturbation bound (1.2) necessarily implies*

$$\|P - Q\| < 1 ? \quad (1.3)$$

Our guess is that the answer to the question (i) should be positive, but at the moment this is only a conjecture.

Notice that the quantity $\theta = \arcsin(\|P - Q\|)$ expresses the maximal angle between the ranges $\text{Ran}(P)$ and $\text{Ran}(Q)$ of the orthogonal projections P and Q (see Definition 2.1 and Remark 2.2 below). If $\theta < \pi/2$, the subspaces $\text{Ran}(P)$ and $\text{Ran}(Q)$ are said to be in the acute-angle case. Thus, there is an equivalent geometric formulation of the question (i): Does the perturbation bound (1.2) together with the single spectral condition (1.1) always imply that the spectral subspaces of A and L associated with the respective unperturbed and perturbed spectral sets σ and ω are in the acute-angle case?

Furthermore, provided it is established that (1.3) holds, at least for

$$\|V\| < cd \quad (1.4)$$

with some constant $c < 1/2$, another important question arises:

(ii) What function $M(x)$, $x \in [0, c]$, is best possible in the bound

$$\arcsin(\|P - Q\|) \leq M\left(\frac{\|V\|}{d}\right)? \quad (1.5)$$

The estimating function M in (1.5) is required to be universal in the sense that it should be the same for all self-adjoint A and V for which the conditions (1.1) and (1.4) hold.

Note that if one adds to (1.1) an extra assumption that one of the sets σ and Σ lies in a finite or infinite gap of the other set, say, σ lies in a gap of Σ , the answer to the question (i) is known to be positive and the optimal function M in the bound (1.5) is given by $M(x) = \frac{1}{2} \arcsin(2x)$, $x \in [0, \frac{1}{2}]$. This is the essence of the Davis-Kahan sin 2Θ Theorem [11]. For the same particular mutual positions of the spectral sets σ and Σ the positive answer to the question (i) and complete answers to the question (ii) have also been given (under conditions on $\|V\|$ much weaker than (1.2)) in the case where the perturbation V is off-diagonal with respect to the partition $\text{spec}(A) = \sigma \cup \Sigma$ (see the tan 2Θ Theorem in [11] and the a priori tan Θ Theorem in [4, 21]; cf. the extensions of the tan 2Θ Theorem in [12, 14, 21]).

As for the general case where no requirements are imposed on the spectral sets σ and Σ except for the separation condition (1.1) and no assumptions are made on the structure of the perturbation V , we are only aware of the partial answers to the questions (i) and (ii) found in [16] and [19]. We underline that both [16] and [19] only treat the case where the unperturbed operator A is bounded. In [16] it was proven that inequality (1.3) holds true whenever $\|V\| < c_{\text{KMM}} d$ with

$$c_{\text{KMM}} = \frac{2}{2 + \pi} = 0.388984\dots \quad (1.6)$$

In [19] the value of c in the bound (1.4) ensuring (1.3) has been raised to

$$c_{\text{MS}} = \frac{1}{2} - \frac{1}{2e^2} = 0.432332\dots \quad (1.7)$$

Explicit expressions for the corresponding estimating functions M found in [19] and [16] are given below in Remarks 3.6 and 3.8, respectively. The bound of the form (1.5) established in [19] is stronger than its predecessor in [16].

In the present work, the requirement that the operator A should be bounded is withdrawn. Introducing the sequence

$$\varkappa_n = \frac{1}{2} \left(1 - \frac{(\pi^2 - 4)^n}{(\pi^2 + 4)^n} \right), \quad n \in \{0\} \cup \mathbb{N},$$

we prove that under conditions (1.1) and (1.2) the following estimate of the form (1.5) holds:

$$\arcsin(\|P - Q\|) \leq M_*(\frac{\|V\|}{d}), \quad (1.8)$$

where the estimating function $M_*(x)$, $x \in [0, \frac{1}{2}]$, is given by

$$M_*(x) = \frac{1}{2} n_*(x) \arcsin\left(\frac{4\pi}{\pi^2 + 4}\right) + \frac{1}{2} \arcsin\left(\frac{\pi(x - \varkappa_{n_*(x)})}{1 - 2\varkappa_{n_*(x)}}\right), \quad (1.9)$$

with $n_\#(x) = \max \{n \mid n \in \{0\} \cup \mathbb{N}, \varkappa_n \leq x\}$. The estimate (1.8) is sharper than the best previously known bound for $\|P - Q\|$ from [19] (see Remark 5.5 for details). Furthermore, this estimate implies that $\|P - Q\| < 1$ and, thus, that the spectral subspaces $\text{Ran}(P)$ and $\text{Ran}(Q)$ are in the acute-angle case whenever $\|V\| < c_* d$, where the constant

$$c_* = 16 \frac{\pi^6 - 2\pi^4 + 32\pi^2 - 32}{(\pi^2 + 4)^4} = 0.454169\dots \quad (1.10)$$

is larger (and, hence, closer to the desired 1/2) than the best previous constant (1.7).

The plan of the paper is as follows. In Section 2 we recall the notion of maximal angle between subspaces of a Hilbert space and recollect necessary definitions and facts on pairs of subspaces. In Section 3 we extend the best previously known subspace perturbation bound (from [19]) to the case where the unperturbed operator A is already allowed to be unbounded. Note that the extended bound is later on used in the proof of the estimate (1.8). Section 4 is devoted to deriving two new estimates for the variation of a spectral subspace that we call the a priori and a posteriori generic $\sin 2\theta$ bounds. These respective estimates involve the maximal angle between a reducing subspace of the perturbed operator L and a spectral subspace of the unperturbed operator A or vice versa. The principal result of the present work, the estimate (1.8), is proven in Section 5 (see Theorem 5.4). Under the assumption that $V \neq 0$, the proof is performed by multiply employing the a priori generic $\sin 2\theta$ bound and using, step by step, the triangle inequality for the maximal angles between the corresponding spectral subspaces of the operator A and two consecutive intermediate operators $L_j = A + t_j V$, where $t_j = \varkappa_j d / \|V\|$, $j \in \{0\} \cup \mathbb{N}$. Finally, in Section 6 we apply the bound (1.8) to the Schrödinger operator describing a boundedly perturbed N -dimensional isotropic quantum harmonic oscillator.

The following notations are used throughout the paper. By a subspace of a Hilbert space we always mean a closed linear subset. The identity operator on a subspace (or on the whole Hilbert space) \mathfrak{P} is denoted by $I_{\mathfrak{P}}$; if no confusion arises, the index \mathfrak{P} is often omitted. The Banach space of bounded linear operators from a Hilbert space \mathfrak{P} to a Hilbert space \mathfrak{Q} is denoted by $\mathcal{B}(\mathfrak{P}, \mathfrak{Q})$ and by $\mathcal{B}(\mathfrak{P})$ if $\mathfrak{Q} = \mathfrak{P}$. If P is an orthogonal projection in a Hilbert space \mathfrak{H} onto the subspace \mathfrak{P} , by P^\perp we denote the orthogonal projection onto the orthogonal complement $\mathfrak{P}^\perp := \mathfrak{H} \ominus \mathfrak{P}$ of the subspace \mathfrak{P} . The notation $E_T(\sigma)$ is used for the spectral projection of a self-adjoint operator T associated with a Borel set $\sigma \subset \mathbb{R}$. By $\mathcal{O}_r(\sigma)$, $r \geq 0$, we denote the closed r -neighbourhood of σ in \mathbb{R} , i.e. $\mathcal{O}_r(\sigma) = \{x \in \mathbb{R} \mid \text{dist}(x, \sigma) \leq r\}$.

2. Preliminaries

The main purpose of this section is to recollect relevant facts on a pair of subspaces and the maximal angle between them.

It is well known that if \mathfrak{H} is a Hilbert space then $\|P - Q\| \leq 1$ for any two orthogonal projections P and Q in \mathfrak{H} (see, e.g., [1, Section 34]). We start with the following definition.

Definition 2.1. Let \mathfrak{P} and \mathfrak{Q} be subspaces of the Hilbert space \mathfrak{H} and P and Q the orthogonal projections in \mathfrak{H} with $\text{Ran}(P) = \mathfrak{P}$ and $\text{Ran}(Q) = \mathfrak{Q}$. The quantity

$$\theta(\mathfrak{P}, \mathfrak{Q}) := \arcsin(\|P - Q\|)$$

is called the *maximal angle* between the subspaces \mathfrak{P} and \mathfrak{Q} .

Remark 2.2. The concept of maximal angle between subspaces is traced back to M.G. Krein, M. A. Krasnoselsky, and D. P. Milman [17]. Assuming that $(\mathfrak{P}, \mathfrak{Q})$ is an ordered pair of subspaces with $\mathfrak{P} \neq \{0\}$, they applied the notion of the (relative) maximal angle between \mathfrak{P} and \mathfrak{Q} to the number φ in $[0, \frac{\pi}{2}]$ introduced by

$$\sin \varphi(\mathfrak{P}, \mathfrak{Q}) = \sup_{x \in \mathfrak{P}, \|x\|=1} \text{dist}(x, \mathfrak{Q}).$$

If both $\mathfrak{P} \neq \{0\}$ and $\mathfrak{Q} \neq \{0\}$ then

$$\theta(\mathfrak{P}, \mathfrak{Q}) = \max\{\varphi(\mathfrak{P}, \mathfrak{Q}), \varphi(\mathfrak{Q}, \mathfrak{P})\}$$

(see, e.g., [8, Example 3.5]) and, in general, $\varphi(\mathfrak{P}, \mathfrak{Q}) \neq \varphi(\mathfrak{Q}, \mathfrak{P})$. Unlike $\varphi(\mathfrak{P}, \mathfrak{Q})$, the maximal angle $\theta(\mathfrak{P}, \mathfrak{Q})$ is always symmetric with respect to the interchange of the arguments \mathfrak{P} and \mathfrak{Q} . Furthermore,

$$\varphi(\mathfrak{Q}, \mathfrak{P}) = \varphi(\mathfrak{P}, \mathfrak{Q}) = \theta(\mathfrak{Q}, \mathfrak{P}) \quad \text{whenever } \|P - Q\| < 1.$$

Remark 2.3. The distance function $d(\mathfrak{P}, \mathfrak{Q}) = \|P - Q\|$ is a natural metric on the set $\mathcal{S}(\mathfrak{H})$ of all subspaces of the Hilbert space \mathfrak{H} . Clearly, for the maximal angle $\theta(\mathfrak{P}, \mathfrak{Q})$ to be another metric on $\mathcal{S}(\mathfrak{H})$, only the triangle inequality

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq \theta(\mathfrak{P}, \mathfrak{R}) + \theta(\mathfrak{R}, \mathfrak{Q}), \quad \text{for any } \mathfrak{P}, \mathfrak{Q}, \mathfrak{R} \in \mathcal{S}(\mathfrak{H}),$$

is needed to be proven. That $\theta(\mathfrak{P}, \mathfrak{Q})$ is indeed a metric on $\mathcal{S}(\mathfrak{H})$ has been shown in [9]. In Lemma 2.15 below we will give an alternative proof of this fact.

Remark 2.4. $\theta(\mathfrak{P}^\perp, \mathfrak{Q}^\perp) = \theta(\mathfrak{P}, \mathfrak{Q})$. This follows from the equalities

$$\|P^\perp - Q^\perp\| = \|(I - P) - (I - Q)\| = \|P - Q\|,$$

where I is the identity operator on \mathfrak{H} .

Definition 2.5. Two subspaces \mathfrak{P} and \mathfrak{Q} of the Hilbert space \mathfrak{H} are said to be in the *acute-angle case* if $\mathfrak{P} \neq \{0\}$, $\mathfrak{Q} \neq \{0\}$, and $\theta(\mathfrak{P}, \mathfrak{Q}) < \frac{\pi}{2}$, that is, if

$$\|P - Q\| < 1, \tag{2.1}$$

where P and Q are the orthogonal projections in \mathfrak{H} with $\text{Ran}(P) = \mathfrak{P}$ and $\text{Ran}(Q) = \mathfrak{Q}$.

Remark 2.6. We recall that the subspaces \mathfrak{P} and \mathfrak{Q} are said to be in the *acute case* if $\mathfrak{P} \cap \mathfrak{Q}^\perp = \mathfrak{P}^\perp \cap \mathfrak{Q} = \{0\}$ (cf., e.g., [11, Definition 3.1]). The bound $\|P - Q\| < 1$ implies both $\mathfrak{P} \cap \mathfrak{Q}^\perp = \{0\}$ and $\mathfrak{P}^\perp \cap \mathfrak{Q} = \{0\}$ (see, e.g., [15, Theorem 2.2]). Hence, if the subspaces \mathfrak{P} and \mathfrak{Q} are in the acute-angle case, they are automatically in the acute case.

Remark 2.7. It is known (see, e.g., [15, Corollary 3.4]) that inequality (2.1) holds true (and, thus, \mathfrak{P} and \mathfrak{Q} are in the acute-angle case) if and only if the subspace \mathfrak{Q} is the graph of a bounded linear operator X from the subspace \mathfrak{P} to its orthogonal complement \mathfrak{P}^\perp , i.e.

$$\mathfrak{Q} = \mathcal{G}(X) := \{x \oplus Xx \mid x \in \mathfrak{P}\}. \quad (2.2)$$

In such a case the projection Q admits the representation

$$Q = \begin{pmatrix} (I_{\mathfrak{P}} + X^*X)^{-1} & (I_{\mathfrak{P}} + X^*X)^{-1}X^* \\ X(I_{\mathfrak{P}} + X^*X)^{-1} & X(I_{\mathfrak{P}} + X^*X)^{-1}X^* \end{pmatrix} \quad (2.3)$$

with respect the orthogonal decomposition $\mathfrak{H} = \mathfrak{P} \oplus \mathfrak{P}^\perp$ (cf. [15, Remark 3.6]). Moreover, under condition (2.1) the orthogonal projections P and Q are unitarily equivalent. In particular,

$$P = U^*QU,$$

where the unitary operator U is given by

$$U = \begin{pmatrix} (I_{\mathfrak{P}} + X^*X)^{-1/2} & -X^*(I_{\mathfrak{P}^\perp} + XX^*)^{-1/2} \\ X(I_{\mathfrak{P}} + X^*X)^{-1/2} & (I_{\mathfrak{P}^\perp} + XX^*)^{-1/2} \end{pmatrix}. \quad (2.4)$$

Remark 2.8. One verifies by inspection that the unitary operator (2.4) possesses the remarkable properties

$$U^2 = (Q^\perp - Q)(P^\perp - P) \quad \text{and} \quad \operatorname{Re} U > 0, \quad (2.5)$$

where $\operatorname{Re} U = \frac{1}{2}(U + U^*)$ denotes the real part of U .

The concept of direct rotation from one subspace in the Hilbert space to another was suggested by C. Davis in [10]. The idea of this concept goes back yet to B. Sz.-Nagy (see [22, §105]) and T. Kato (see [13, Sections I.4.6 and I.6.8]). We adopt the following definition of direct rotation (see [11, Proposition 3.3]; cf. [21, Definition 2.12]).

Definition 2.9. Let \mathfrak{P} and \mathfrak{Q} be subspaces of the Hilbert space \mathfrak{H} . A unitary operator S on \mathfrak{H} is called the *direct rotation* from \mathfrak{P} to \mathfrak{Q} if

$$QS = SP, \quad S^2 = (Q^\perp - Q)(P^\perp - P), \quad \text{and} \quad \operatorname{Re} S \geq 0, \quad (2.6)$$

where P and Q are the orthogonal projections in \mathfrak{H} such that $\operatorname{Ran}(P) = \mathfrak{P}$ and $\operatorname{Ran}(Q) = \mathfrak{Q}$.

Remark 2.10. If the subspaces \mathfrak{P} and \mathfrak{Q} are not in the acute case, the direct rotation from \mathfrak{P} to \mathfrak{Q} exists if and only if

$$\dim(\mathfrak{P} \cap \mathfrak{Q}^\perp) = \dim(\mathfrak{Q} \cap \mathfrak{P}^\perp)$$

(see [11, Proposition 3.2]). If it exists, it is not unique.

Remark 2.11. If the subspaces \mathfrak{P} and \mathfrak{Q} are in the acute case then there exists a unique direct rotation from \mathfrak{P} to \mathfrak{Q} (see [11, Propositions 3.1 and 3.3] or [21, Theorem 2.14]). Comparing (2.5) with (2.6), one concludes that the unitary operator U

given by (2.4) represents the unique direct rotation from the subspace \mathfrak{P} to the subspace \mathfrak{Q} whenever these subspaces are in the acute-angle case. The direct rotation U has the extremal property (see [10, Theorem 7.1])

$$\|U - I_{\mathfrak{H}}\| = \inf_{\tilde{U} \in \mathcal{U}(\mathfrak{P}, \mathfrak{Q})} \|\tilde{U} - I_{\mathfrak{H}}\|, \quad (2.7)$$

where $\mathcal{U}(\mathfrak{P}, \mathfrak{Q})$ denotes the set of all unitary operators \tilde{U} on \mathfrak{H} such that $P = \tilde{U}^* Q \tilde{U}$. Equality (2.7) says that the direct rotation U is norm closest to the identity operator among all unitary operators on \mathfrak{H} mapping \mathfrak{P} onto \mathfrak{Q} .

The operator X in the graph representation (2.2) is usually called the *angular operator* for the (ordered) pair of the subspaces \mathfrak{P} and \mathfrak{Q} . The usage of this term is motivated by the equality (see, e.g., [15])

$$\Theta(\mathfrak{P}, \mathfrak{Q}) = \arctan \sqrt{X^* X}, \quad (2.8)$$

where $\Theta(\mathfrak{P}, \mathfrak{Q})$ denotes the *operator angle* between the subspaces \mathfrak{P} and \mathfrak{Q} (measured relative to the subspace \mathfrak{P}). One verifies by inspection (see, e.g., [15, Corollary 3.4]) that, in the acute-angle case,

$$\sin(\theta(\mathfrak{P}, \mathfrak{Q})) \equiv \|P - Q\| = \frac{\|X\|}{\sqrt{1 + \|X\|^2}} = \sin \|\Theta(\mathfrak{P}, \mathfrak{Q})\|, \quad (2.9)$$

which means, in particular, that

$$\theta(\mathfrak{P}, \mathfrak{Q}) = \|\Theta(\mathfrak{P}, \mathfrak{Q})\|. \quad (2.10)$$

Furthermore, the lower bound for the spectrum of the real part of the direct rotation (2.4) is given by (cf. [21, Remark 2.18])

$$\min(\text{spec}(\text{Re } U)) = \frac{1}{\sqrt{1 + \|X\|^2}} = \cos(\theta(\mathfrak{P}, \mathfrak{Q})). \quad (2.11)$$

To have a more convenient characterization of the distinction between a unitary operator and the identity one, we recall the notion of the spectral angle.

Definition 2.12. Let S be a unitary operator. The number

$$\vartheta(S) = \sup_{z \in \text{spec}(S)} |\arg z|, \quad \arg z \in (-\pi, \pi],$$

is called the *spectral angle* of S .

Remark 2.13. The size of $\|S - I\|$ is easily computed in terms of $\vartheta(S)$ and vice versa (see [21, Lemma 2.19]). In particular,

$$\|S - I\| = 2 \sin \left(\frac{\vartheta(S)}{2} \right). \quad (2.12)$$

Furthermore,

$$\cos \vartheta(S) = \min(\text{spec}(\text{Re } S)). \quad (2.13)$$

By comparing (2.11) with (2.13) and (2.7) with (2.12) we immediately arrive at the following assertion.

Proposition 2.14. Let \mathfrak{P} and \mathfrak{Q} be subspaces of a Hilbert space \mathfrak{H} . Assume that \mathfrak{P} and \mathfrak{Q} are in the acute-angle case. Then:

- (i) *The maximal angle between \mathfrak{P} and \mathfrak{Q} is nothing but the spectral angle of the direct rotation U from \mathfrak{P} to \mathfrak{Q} , i.e., $\theta(\mathfrak{P}, \mathfrak{Q}) = \vartheta(U)$.*
- (ii) *$\vartheta(S) \geq \theta(\mathfrak{P}, \mathfrak{Q})$ for any unitary S on \mathfrak{H} mapping \mathfrak{P} onto \mathfrak{Q} .*

We conclude the present section with a proof of the triangle inequality for the maximal angles between subspaces.

Lemma 2.15. *Let \mathfrak{P} , \mathfrak{Q} , and \mathfrak{R} be three arbitrary subspaces of the Hilbert space \mathfrak{H} . The following inequality holds:*

$$\theta(\mathfrak{P}, \mathfrak{Q}) \leq \theta(\mathfrak{P}, \mathfrak{R}) + \theta(\mathfrak{R}, \mathfrak{Q}). \quad (2.14)$$

Proof. If $\theta(\mathfrak{P}, \mathfrak{R}) + \theta(\mathfrak{R}, \mathfrak{Q}) \geq \pi/2$, inequality (2.14) holds true since $\theta(\mathfrak{P}, \mathfrak{Q}) \leq \pi/2$ by the definition of the maximal angle.

Suppose that $\theta(\mathfrak{P}, \mathfrak{R}) + \theta(\mathfrak{R}, \mathfrak{Q}) < \pi/2$. In such a case both the pairs $(\mathfrak{P}, \mathfrak{R})$ and $(\mathfrak{R}, \mathfrak{Q})$ of the argument subspaces are in the acute-angle case. Then there are a unique direct rotation U_1 from \mathfrak{P} to \mathfrak{R} and a unique direct rotation U_2 from \mathfrak{R} to \mathfrak{Q} (see Remark 2.11). By [21, Lemma 2.22], the spectral angle $\vartheta(S)$ of the product $S := U_2 U_1$ of the unitary operators U_1 and U_2 satisfies the bound

$$\vartheta(S) \leq \vartheta(U_1) + \vartheta(U_2). \quad (2.15)$$

Notice that by Proposition 2.14 (i)

$$\vartheta(U_1) = \theta(\mathfrak{P}, \mathfrak{R}) \text{ and } \vartheta(U_2) = \theta(\mathfrak{R}, \mathfrak{Q}), \quad (2.16)$$

because both U_1 and U_2 are direct rotations. Since $\text{Ran}(U_1|_{\mathfrak{P}}) = \mathfrak{Q}$ and $\text{Ran}(U_2|_{\mathfrak{Q}}) = \mathfrak{R}$, the unitary operator S maps \mathfrak{P} onto \mathfrak{Q} . Hence, $\vartheta(S) \geq \theta(\mathfrak{P}, \mathfrak{Q})$ by Proposition 2.14 (ii). Combining this with (2.15) and (2.16) completes the proof. \square

3. An extension of the best previously known bound

In this section we extend the norm estimate on variation of spectral subspaces of a bounded self-adjoint operator A under a bounded self-adjoint perturbation V established recently by K. A. Makarov and A. Seelmann in [19] to the case where A is allowed to be unbounded.

We begin with recalling the concept of a strong solution to the operator Sylvester equation.

Definition 3.1. Let Λ_0 and Λ_1 be (possibly unbounded) self-adjoint operators on the Hilbert spaces \mathfrak{H}_0 and \mathfrak{H}_1 , respectively, and $Y \in \mathcal{B}(\mathfrak{H}_0, \mathfrak{H}_1)$. A bounded operator $X \in \mathcal{B}(\mathfrak{H}_0, \mathfrak{H}_1)$ is said to be a *strong solution* to the Sylvester equation

$$X\Lambda_0 - \Lambda_1 X = Y \quad (3.1)$$

if

$$\text{Ran}(X|_{\text{Dom}(\Lambda_0)}) \subset \text{Dom}(\Lambda_1)$$

and

$$X\Lambda_0 f - \Lambda_1 X f = Y f \quad \text{for all } f \in \text{Dom}(\Lambda_0).$$

We will use the following well known result on a sharp norm bound for strong solutions to operator Sylvester equations (cf. [5, Theorem 4.9 (i)]).

Theorem 3.2. *Let Λ_0 , Λ_1 , and Y be as in Definition 3.1. If the spectra of Λ_0 and Λ_1 are disjoint, i.e. if*

$$\delta := \text{dist}(\text{spec}(\Lambda_0), \text{spec}(\Lambda_1)) > 0,$$

then the Sylvester equation (3.1) has a unique strong solution $X \in \mathcal{B}(\mathfrak{H}_0, \mathfrak{H}_1)$. Moreover, the solution X satisfies the bound

$$\|X\| \leq \frac{\pi}{2} \frac{\|Y\|}{\delta}. \quad (3.2)$$

Remark 3.3. The fact that the constant c in the estimate $\delta\|X\| \leq c\|Y\|$ for the generic disposition of the spectra of Λ_0 and Λ_1 is not greater than $\pi/2$ goes back to B. Sz.-Nagy and A. Strausz (see [23]). The sharpness of the value $c = \pi/2$ has been proven by R. McEachin [20]. In its present form the statement is obtained by combining [2, Theorem 2.7] and [3, Lemma 4.2].

The next statement represents nothing but a corollary to Theorem 3.2.

Proposition 3.4. (cf. [20]) *Let A and B be possibly unbounded self-adjoint operators on the Hilbert space \mathfrak{H} with the same domain, i.e. $\text{Dom}(B) = \text{Dom}(A)$. Assume that the closure $C = \overline{B - A}$ of the symmetric operator $B - A$ is a bounded self-adjoint operator on \mathfrak{H} . Then for any two Borel sets $\omega, \Omega \subset \mathbb{R}$ the following inequality holds:*

$$\text{dist}(\omega, \Omega) \|E_A(\omega)E_B(\Omega)\| \leq \frac{\pi}{2} \|C\|, \quad (3.3)$$

where $E_A(\omega)$ and $E_B(\Omega)$ are the spectral projections of A and B associated with the sets ω and Ω , respectively.

Proof. Clearly, it suffices to give a proof only for the case where

$$\omega \subset \text{spec}(A), \quad \Omega \subset \text{spec}(B), \quad \text{and} \quad \text{dist}(\omega, \Omega) > 0. \quad (3.4)$$

Assuming (3.4), we set $P = E_A(\omega)$ and $Q = E_B(\Omega)$. The spectral theorem implies

$$Pf \in \text{Dom}(A) \cap \mathfrak{P} \quad \text{for any } f \in \text{Dom}(A), \quad (3.5)$$

$$Qg \in \text{Dom}(B) \cap \mathfrak{Q} \quad \text{for any } g \in \text{Dom}(B), \quad (3.6)$$

where $\mathfrak{P} := \text{Ran}(P)$ and $\mathfrak{Q} := \text{Ran}(Q)$ are the spectral subspaces of the operators A and B associated with their respective spectral subsets ω and Ω . Due to $\text{Dom}(B) = \text{Dom}(A)$ the inclusions (3.5) and (3.6) yield

$$\text{Ran}(PQ|_{\text{Dom}(B)}) \subset \text{Dom}(A) \cap \mathfrak{P}. \quad (3.7)$$

Since P commutes with A , Q commutes with B , $P^2 = P$, and $Q^2 = Q$, from (3.5)–(3.7) it follows that

$$PQQBQf - PAP PQf = PCQf \quad \text{for any } f \in \text{Dom}(B). \quad (3.8)$$

Now let A_ω and B_Ω be the parts of the self-adjoint operators A and B associated with their spectral subspaces $\mathfrak{P} = \text{Ran}(P)$ and $\mathfrak{Q} = \text{Ran}(Q)$. That is,

$$A_\omega = A|_{\mathfrak{P}} \quad \text{with} \quad \text{Dom}(A_\omega) = \mathfrak{P} \cap \text{Dom}(A), \quad (3.9)$$

$$B_\Omega = B|_{\mathfrak{Q}} \quad \text{with} \quad \text{Dom}(B_\Omega) = \mathfrak{Q} \cap \text{Dom}(B) \quad (= \mathfrak{Q} \cap \text{Dom}(A)). \quad (3.10)$$

Also set $X := P|_{\mathfrak{Q}} = PQ|_{\mathfrak{Q}}$. Taking into account (3.7), (3.9), and (3.10) we have

$$\text{Ran}(X|_{\text{Dom}(B_\Omega)}) \subset \text{Dom}(A_\omega)$$

and then (3.8) implies

$$XB_\Omega f - A_\omega X f = PCf \quad \text{for any } f \in \text{Dom}(B_\Omega),$$

which means that the operator X is a strong solution to the operator Sylvester equation

$$XB_\Omega - A_\omega X = PC|_{\mathfrak{Q}}.$$

To prove (3.3) it only remains to notice that

$$\begin{aligned} \|\mathbb{E}_A(\omega)\mathbb{E}_B(\Omega)\| &= \|PQ\| = \|X\|, \\ \text{spec}(A_\omega) &= \omega, \quad \text{spec}(B_\Omega) = \Omega, \quad \|PC|_{\mathfrak{Q}}\| \leq \|C\| \end{aligned}$$

and then to apply Theorem 3.2. \square

Theorem 3.5. *Given a (possibly unbounded) self-adjoint operator A on the Hilbert space \mathfrak{H} , assume that a Borel set $\sigma \subset \mathbb{R}$ is an isolated component of the spectrum of A , that is, $\sigma \subset \text{spec}(A)$ and*

$$\text{dist}(\sigma, \Sigma) = d > 0, \quad (3.11)$$

where $\Sigma = \text{spec}(A) \setminus \sigma$. Assume, in addition, that V is a bounded self-adjoint operator on \mathfrak{H} such that

$$\|V\| < d/2 \quad (3.12)$$

and let $\Gamma(t)$, $t \in [0, 1]$, be the spectral projection of the self-adjoint operator

$$L_t = A + tV, \quad \text{Dom}(L_t) = \text{Dom}(A), \quad (3.13)$$

associated with the closed $\|V\|$ -neighborhood $\mathcal{O}_{\|V\|}(\sigma)$ of the set σ . The projection family $\{\Gamma(t)\}_{t \in [0, 1]}$ is norm continuous on the interval $[0, 1]$ and

$$\arcsin(\|\Gamma(b) - \Gamma(a)\|) \leq \frac{\pi}{4} \log \left(\frac{d - 2a\|V\|}{d - 2b\|V\|} \right) \quad \text{whenever } 0 \leq a < b \leq 1. \quad (3.14)$$

Proof. Let $\omega_t = \text{spec}(L_t) \cap \mathcal{O}_{\|V\|}(\sigma)$ and $\Omega_t = \text{spec}(L_t) \cap \mathcal{O}_{\|V\|}(\Sigma)$, $t \in [0, 1]$. Since A is a self-adjoint operator and L_t is given by (3.13), we have

$$\omega_t \cap \Omega_t = \emptyset, \quad \text{spec}(L_t) = \omega_t \cup \Omega_t,$$

and, in fact,

$$\omega_t \subset \mathcal{O}_{t\|V\|}(\sigma) \quad \text{and} \quad \Omega_t \subset \mathcal{O}_{t\|V\|}(\Sigma), \quad t \in [0, 1]. \quad (3.15)$$

Notice that under condition (3.12) from (3.11) and (3.15) it follows that, for $s, t \in [0, 1]$,

$$\text{dist}(\omega_t, \Omega_s) \geq d - t\|V\| - s\|V\| = d - \|V\|(t + s). \quad (3.16)$$

In particular,

$$d - \|V\|(t + s) \geq d - 2\|V\| > 0 \quad \text{whenever } s, t \in [0, 1]. \quad (3.17)$$

Obviously, $\Gamma(t) = \mathsf{E}_{L_t}(\omega_t)$ and $\Gamma(t)^\perp = \mathsf{E}_{L_t}(\Omega_t)$, $t \in [0, 1]$. Thus, for any $s, t \in [0, 1]$ Proposition 3.4 implies

$$\|\Gamma(s)\Gamma(t)^\perp\| \leq \frac{\pi}{2} \frac{\|V\||t-s|}{\text{dist}(\omega_s, \Omega_t)} \quad \text{and} \quad \|\Gamma(s)^\perp\Gamma(t)\| \leq \frac{\pi}{2} \frac{\|V\||t-s|}{\text{dist}(\Omega_s, \omega_t)}. \quad (3.18)$$

Since $\|\Gamma(t) - \Gamma(s)\| = \max\{\|\Gamma(t)\Gamma(s)^\perp\|, \|\Gamma(t)^\perp\Gamma(s)\|\}$, from (3.16) and (3.18) one concludes that

$$\|\Gamma(t) - \Gamma(s)\| \leq \frac{\pi}{2} \frac{\|V\||t-s|}{d - \|V\|(t+s)} \quad \text{for any } s, t \in [0, 1]. \quad (3.19)$$

In view of (3.17), the operator norm continuity of the projection path $\{\Gamma(t)\}_{t \in [0,1]}$ on the interval $[0, 1]$ follows immediately from estimate (3.19).

Now suppose that $s < t$ (as before, $s, t \in [0, 1]$) and observe that

$$\frac{t-s}{d - \|V\|(t+s)} < \int_s^t \frac{d\tau}{d - 2\|V\|\tau}. \quad (3.20)$$

Indeed, the difference between the right-hand side and left-hand side parts of (3.20) may be written as

$$\int_s^{\tau_c} (f(\tau) + f(2\tau_c - \tau) - 2f(\tau_c)) d\tau, \quad (3.21)$$

where $\tau_c = (s+t)/2$ is the center of the interval $[s, t]$ and

$$f(\tau) := \frac{1}{d - 2\|V\|\tau}, \quad \tau \in [s, t].$$

One verifies by inspection that the expression $f(\tau) + f(2\tau_c - \tau) - 2f(\tau_c)$ under the integration sign in (3.21) is strictly positive for $\tau \in [s, \tau_c]$ and zero for $\tau = \tau_c$. Therefore, the integral in (3.21) is positive and hence inequality (3.20) holds true.

Assume that $0 \leq a < b \leq 1$. For a sequence of points $t_0, t_1, \dots, t_n \in [a, b]$, $n \in \mathbb{N}$, such that

$$a = t_0 < t_1 < \dots < t_n = b \quad (3.22)$$

by (3.19) and (3.20) one obtains

$$\begin{aligned} \sum_{j=0}^{n-1} \|\Gamma(t_{j+1}) - \Gamma(t_j)\| &\leq \frac{\pi\|V\|}{2} \sum_{j=0}^{n-1} \frac{t_{j+1} - t_j}{d - \|V\|(t_j + t_{j+1})} \\ &< \frac{\pi\|V\|}{2} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{d\tau}{d - 2\|V\|\tau} \\ &= \frac{\pi\|V\|}{2} \int_a^b \frac{d\tau}{d - 2\|V\|\tau}. \end{aligned} \quad (3.23)$$

Evaluating the last integral in (3.23) and taking supremum over all choices of $n \in \mathbb{N}$ and $t_0, t_1, \dots, t_n \in [a, b]$ satisfying (3.22) results in the bound

$$\ell(\Gamma) \leq \frac{\pi}{4} \log \left(\frac{d - 2a\|V\|}{d - 2b\|V\|} \right),$$

where

$$\ell(\Gamma) := \sup \left\{ \sum_{j=0}^{n-1} \|\Gamma(t_{j+1}) - \Gamma(t_j)\| \mid n \in \mathbb{N}, a = t_0 < t_1 < \dots < t_n = b \right\} \quad (3.24)$$

is the length of the (continuous) projection path $\Gamma(t)$, $t \in [a, b]$. Applying [19, Corollary 4.2], which establishes that $\arcsin(\|\Gamma(b) - \Gamma(a)\|) \leq \ell(\Gamma)$, completes the proof. \square

Remark 3.6. Let $\mathfrak{A} = \text{Ran}(E_A(\sigma))$ and $\mathfrak{L} = \text{Ran}(E_L(\omega))$ where $L := A + V$ with $\text{Dom}(L) = \text{Dom}(A)$ and $\omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\sigma)$. By setting $a = 0$ and $b = 1$ in (3.14), one obtains

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_{\text{MS}} \left(\frac{\|V\|}{d} \right), \quad (3.25)$$

where $\theta(\mathfrak{A}, \mathfrak{L})$ is the maximal angle between the spectral subspaces \mathfrak{A} and \mathfrak{L} and

$$M_{\text{MS}}(x) := \frac{\pi}{4} \log \left(\frac{1}{1-2x} \right), \quad x \in [0, \frac{1}{2}). \quad (3.26)$$

For bounded A , the estimate (3.25) has been established in [19, Theorem 6.1].

Note that (3.25) implies that $\theta(\mathfrak{A}, \mathfrak{L}) < \frac{\pi}{2}$ and, thus, that the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case if

$$\|V\| < c_{\text{MS}} d, \quad (3.27)$$

where c_{MS} is given by (1.7).

Remark 3.7. For future references we remark that, due to (3.25),

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq \frac{\pi}{4} \quad \text{whenever } \|V\| \leq c_{\pi/4} d, \quad (3.28)$$

where

$$c_{\pi/4} = \frac{1}{2} - \frac{1}{2e} = 0.316060\dots \quad (3.29)$$

Remark 3.8. The bound (3.25) is stronger than the earlier estimate [16]

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_{\text{KMM}} \left(\frac{\|V\|}{d} \right) \quad \left(< \frac{\pi}{2} \right) \quad \text{if } \|V\| < c_{\text{KMM}} d, \quad (3.30)$$

where the value of c_{KMM} is given by (1.6) and

$$M_{\text{KMM}}(x) := \arcsin \left(\frac{\pi x}{2(1-x)} \right), \quad 0 \leq x \leq c_{\text{KMM}}. \quad (3.31)$$

The estimate (3.30) was established in the proof of Lemma 2.2 in [16].

4. A priori and a posteriori generic $\sin 2\theta$ estimates

We begin this section with the proof of an estimate for $\sin(2\theta(\mathfrak{A}, \mathfrak{L}))$, where \mathfrak{A} is a reducing subspace of the self-adjoint operator A and \mathfrak{L} is the spectral subspace of the boundedly perturbed self-adjoint operator $L = A + V$. In general, \mathfrak{A} does not need to be a spectral subspace of A .

Theorem 4.1. *Let A be a (possibly unbounded) self-adjoint operator on the Hilbert space \mathfrak{H} . Suppose that V is a bounded self-adjoint operator on \mathfrak{H} and $L = A + V$ with $\text{Dom}(L) = \text{Dom}(A)$. Assume that \mathfrak{A} is a reducing subspace of A and \mathfrak{L} is a spectral subspace of L associated with a Borel subset ω of its spectrum. If the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case then*

$$\text{dist}(\omega, \Omega) \sin(2\theta) \leq \pi \|V\|, \quad (4.1)$$

where $\Omega = \text{spec}(L) \setminus \omega$ is the remainder of the spectrum of L and $\theta := \theta(\mathfrak{A}, \mathfrak{L})$ denotes the maximal angle between \mathfrak{A} and \mathfrak{L} .

Proof. For $\text{dist}(\omega, \Omega) = 0$ the bound (4.1) is trivial. Throughout the proof below we will assume that $\text{dist}(\omega, \Omega) \neq 0$.

Since \mathfrak{A} is a reducing subspace of the self-adjoint operator A , its orthogonal complement $\mathfrak{A}^\perp = \mathfrak{H} \ominus \mathfrak{A}$ is also a reducing subspace of A . Furthermore, $\text{Dom}(A) = \text{Dom}(A_0) \oplus \text{Dom}(A_1)$, where $\text{Dom}(A_0)$ and $\text{Dom}(A_1)$ are domains of the parts $A_0 = A|_{\mathfrak{A}}$ and $A_1 = A|_{\mathfrak{A}^\perp}$ of A in its reducing subspaces \mathfrak{A} and \mathfrak{A}^\perp , respectively (see, e.g., [7, Section 3.6]).

Let P be the orthogonal projection in \mathfrak{H} onto the subspace \mathfrak{A} . Since $V \in \mathcal{B}(\mathfrak{H})$, the (self-adjoint) operator L admits the following block representation with respect to the orthogonal decomposition $\mathfrak{H} = \mathfrak{A} \oplus \mathfrak{A}^\perp$:

$$L = \begin{pmatrix} D_0 & B \\ B^* & D_1 \end{pmatrix}, \quad \text{Dom}(L) = \text{Dom}(D_0) \oplus \text{Dom}(D_1) \quad (= \text{Dom}(A)), \quad (4.2)$$

where $B = PV|_{\mathfrak{A}^\perp}$, $D_0 = A_0 + PV|_{\mathfrak{A}}$, with $\text{Dom}(D_0) = \text{Dom}(A_0)$ and $D_1 = A_1 + P^\perp V|_{\mathfrak{A}^\perp}$, with $\text{Dom}(D_1) = \text{Dom}(A_1)$.

That the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case implies that there is a bounded operator X from \mathfrak{A} to \mathfrak{A}^\perp such that \mathfrak{L} is the graph of X , that is, $\mathfrak{L} = \mathcal{G}(X)$ (see Remark 2.7). It is well known (see, e.g., [2, Lemma 5.3]) that the graph subspace $\mathcal{G}(X)$ is a reducing subspace for the block operator matrix (4.2) if and only if the angular operator X is a strong solution to the operator Riccati equation

$$XD_0 - D_1 X + XBX = B^*. \quad (4.3)$$

The notion of the strong solution to (4.3) means that (see [2, 3]; cf. Definition 3.1)

$$\text{Ran}(X|_{\text{Dom}(D_0)}) \subset \text{Dom}(D_1) \quad (4.4)$$

and

$$XD_0 f - D_1 X f + XBX f = B^* f \quad \text{for all } f \in \text{Dom}(D_0). \quad (4.5)$$

It is straightforward to verify that if X is a strong solution to (4.5) then

$$XZ_0 f - Z_1 X f = B^*(I + X^* X)f \quad \text{for all } f \in \text{Dom}(D_0), \quad (4.6)$$

where $Z_0 = D_0 + BX$ with $\text{Dom}(Z_0) = \text{Dom}(D_0) = \text{Dom}(A_0)$ and $Z_1 = D_1 - B^* X^*$ with $\text{Dom}(Z_1) = \text{Dom}(D_1) = \text{Dom}(A_1)$.

Our next step is in transforming (4.6) into

$$\begin{aligned} X(I + X^* X)^{-1/2} \Lambda_0 (I + X^* X)^{1/2} f - (I + XX^*)^{-1/2} \Lambda_1 (I + XX^*)^{1/2} X f \\ = B^*(I + X^* X)f \quad \text{for all } f \in \text{Dom}(D_0), \end{aligned} \quad (4.7)$$

where Λ_0 and Λ_1 are given by

$$\begin{aligned}\Lambda_0 &= (I + X^*X)^{1/2}Z_0(I + X^*X)^{-1/2}, \\ \text{Dom}(\Lambda_0) &= \text{Ran}\left((I + X^*X)^{1/2}\Big|_{\text{Dom}(D_0)}\right),\end{aligned}\quad (4.8)$$

and

$$\begin{aligned}\Lambda_1 &= (I + XX^*)^{1/2}Z_1(I + XX^*)^{-1/2}, \\ \text{Dom}(\Lambda_1) &= \text{Ran}\left((I + XX^*)^{1/2}\Big|_{\text{Dom}(D_1)}\right).\end{aligned}\quad (4.9)$$

Note that the (self-adjoint) operator L is unitary equivalent to the block diagonal operator matrix $\Lambda = \text{diag}(\Lambda_0, \Lambda_1)$, $\text{Dom}(\Lambda) = \text{Dom}(\Lambda_0) \oplus \text{Dom}(\Lambda_1)$ (see, e.g., [2, Theorem 5.5]) and, thus, both Λ_0 and Λ_1 are self-adjoint operators. Furthermore, from (4.8) and (4.9) it follows that Z_0 and Z_1 are similar to Λ_0 and Λ_1 , respectively. Combining [2, Theorem 5.5] with [5, Corollary 2.9 (ii)] then yields

$$\text{spec}(\Lambda_0) = \text{spec}(L|_{\mathfrak{L}}) = \omega \quad \text{and} \quad \text{spec}(\Lambda_1) = \text{spec}(L|_{\mathfrak{L}^\perp}) = \Omega. \quad (4.10)$$

Applying $(I + XX^*)^{1/2}$ from the left to both sides of (4.6) and choosing $f = (I + X^*X)^{-1/2}g$ with $g \in \text{Dom}(\Lambda_0)$, we arrive at the Sylvester equation

$$K\Lambda_0 g - \Lambda_1 K g = Y g \quad \text{for all } g \in \text{Dom}(\Lambda_0), \quad (4.11)$$

where

$$K = (I + XX^*)^{1/2}X(I + X^*X)^{-1/2}, \quad (4.12)$$

$$Y = (I + XX^*)^{1/2}B^*(I + X^*X)^{1/2}. \quad (4.13)$$

By (4.8) we have $\text{Ran}\left((I + X^*X)^{-1/2}\Big|_{\text{Dom}(\Lambda_0)}\right) = \text{Dom}(D_0)$. Furthermore,

$$\text{Ran}\left(X\Big|_{\text{Dom}(D_0)}\right) \subset \text{Dom}(D_1)$$

by (4.4), and thus, by (4.9),

$$\text{Ran}\left(K\Big|_{\text{Dom}(\Lambda_0)}\right) \subset \text{Dom}(\Lambda_1). \quad (4.14)$$

Hence K is a strong solution to the Sylvester equation (4.11).

It is easy to verify (see [6, Lemma 2.5]) that $(I + XX^*)^{1/2}X = X(I + X^*X)^{1/2}$. Thus, (4.12) simplifies to nothing but the identity $X = K$, which by (4.11) and (4.14) means that X is a strong solution to the Sylvester equation

$$X\Lambda_0 - \Lambda_1 X = Y. \quad (4.15)$$

Observe that $\|Y\| \leq \|B\|(1 + \|X\|^2)$. Taking into account (4.10), Theorem 3.2 yields

$$\frac{\|X\|}{1 + \|X\|^2} \leq \frac{\pi}{2} \frac{\|B\|}{\text{dist}(\omega, \Omega)}.$$

Now the claim follows from the fact that $2\|X\|/(1 + \|X\|^2) = \sin(2\theta)$ by (2.9). \square

Remark 4.2. Clearly, if $\pi\|V\| > \text{dist}(\omega, \Omega)$, the estimate (4.1) is of no interest. Suppose that $\text{dist}(\omega, \Omega) = \delta > 0$ and $\pi\|V\| \leq \delta$. In such a case (4.1) does allow to obtain a bound for the maximal angle θ but only provided the location of θ relative to $\frac{\pi}{4}$ is known. In particular, if it is known that $\theta \leq \frac{\pi}{4}$ then (4.1) implies the upper

bound $\theta \leq \frac{1}{2} \arcsin\left(\frac{\pi\|V\|}{\delta}\right)$. On the contrary, if it is known that $\theta \geq \frac{\pi}{4}$ then (4.1) yields the lower bound $\theta \geq \frac{\pi}{2} - \frac{1}{2} \arcsin\left(\frac{\pi\|V\|}{\delta}\right)$.

Corollary 4.3. *Let A be a (possibly unbounded) self-adjoint operator on the Hilbert space \mathfrak{H} . Assume that \mathfrak{A} is the spectral subspace of A associated with a Borel subset σ of its spectrum. Suppose that V is a bounded self-adjoint operator on \mathfrak{H} and $L = A + V$ with $\text{Dom}(L) = \text{Dom}(A)$. Furthermore, assume that \mathfrak{L} is a reducing subspace of L . If the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case then*

$$\text{dist}(\sigma, \Sigma) \sin(2\theta) \leq \pi\|V\|, \quad (4.16)$$

where $\Sigma = \text{spec}(A) \setminus \sigma$ is the remainder of the spectrum of A and θ denotes the maximal angle between \mathfrak{A} and \mathfrak{L} .

Proof. Consider A as the perturbation of the operator L , namely view A as $A = L + W$ with $W = -V$, and then the assertion follows from Theorem 4.1. \square

Remark 4.4. Suppose that $\text{dist}(\sigma, \Sigma) = d > 0$ and $\|V\| \leq c_{\pi/4}d$, where $c_{\pi/4}$ is given by (3.29); observe that $c_{\pi/4} < \frac{1}{\pi} = 0.318309\dots$ and, thus, $\frac{\pi\|V\|}{d} < 1$. Let $\omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\sigma)$ and $\mathfrak{L} = \text{Ran}(\mathbf{E}_L(\omega))$. By Remark 3.7 under the condition $\|V\| \leq c_{\pi/4}d$ we have $\theta(\mathfrak{A}, \mathfrak{L}) \leq \frac{\pi}{4}$ and, hence, (4.16) yields the bound (cf. Remark 4.2)

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq \frac{1}{2} \arcsin\left(\frac{\pi\|V\|}{d}\right). \quad (4.17)$$

Notice that

$$\frac{4}{\pi^2 + 4} = 0.288400\dots \quad \text{and} \quad c_{\pi/4} > \frac{4}{\pi^2 + 4}. \quad (4.18)$$

In Theorem 5.4 below we will prove that for $\frac{4}{4+\pi^2}d < \|V\| \leq \frac{1}{\pi}d$ there is a bound on $\theta(\mathfrak{A}, \mathfrak{L})$ tighter than estimate (4.17).

The estimates (4.1) and (4.16) we obtained in Theorem 4.1 and Corollary 4.3 will be called the *generic* a posteriori and a priori $\sin 2\theta$ bounds, respectively. These estimates resemble the corresponding bounds from the celebrated $\sin 2\Theta$ theorems proven by C. Davis and W. M. Kahan in [11, Section 7] for particular dispositions of the sets ω and Ω or σ and Σ . Recall that, when proving the $\sin 2\Theta$ theorems, it is assumed in [11] that the convex hull of one of the sets ω and Ω (resp., the convex hull of one of the sets σ and Σ) does not intersect the other set. An immediately visible difference is that the constant π shows up on the right-hand side parts of the *generic* $\sin 2\theta$ estimates (4.1) and (4.16) instead of the constant 2 in the Davis-Kahan $\sin 2\Theta$ theorems.

5. A new rotation bound by multiply employing $\sin 2\theta$ estimate

Let $\{\varkappa_n\}_{n=0}^\infty$ be a number sequence with

$$\varkappa_0 = 0, \quad \varkappa_n = \frac{4}{\pi^2 + 4} + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_{n-1}, \quad n = 1, 2, \dots. \quad (5.1)$$

One easily verifies that the general term of this sequence reads

$$\varkappa_n = \frac{1 - q^n}{2}, \quad n = 0, 1, 2, \dots, \quad (5.2)$$

with

$$q = \frac{\pi^2 - 4}{\pi^2 + 4} < 1. \quad (5.3)$$

Obviously, the sequence (5.2) is strictly monotonously increasing and it is bounded from above by $1/2$,

$$\varkappa_0 < \varkappa_1 < \varkappa_2 < \dots < \varkappa_n < \dots < 1/2. \quad (5.4)$$

Moreover,

$$\lim_{n \rightarrow \infty} \varkappa_n = 1/2. \quad (5.5)$$

Thus, this sequence produces a countable partition of the interval $[0, \frac{1}{2})$,

$$\left[0, \frac{1}{2}\right) = \bigcup_{n=0}^{\infty} [\varkappa_n, \varkappa_{n+1}). \quad (5.6)$$

Taking into account (5.6), with the sequence $\{\varkappa_n\}_{n=0}^{\infty}$ we associate a function $M_{\star}(x)$, $M_{\star} : [0, \frac{1}{2}) \rightarrow \mathbb{R}$, that is defined separately on each elementary interval $[\varkappa_n, \varkappa_{n+1})$ by

$$M_{\star}(x)|_{[\varkappa_n, \varkappa_{n+1})} = \frac{n}{2} \arcsin\left(\frac{4\pi}{\pi^2 + 4}\right) + \frac{1}{2} \arcsin\left(\frac{\pi(x - \varkappa_n)}{1 - 2\varkappa_n}\right), \quad n = 0, 1, 2, \dots \quad (5.7)$$

We note that the function $M_{\star}(x)$ may be equivalently written in the form (1.9).

Proposition 5.1. *The function $M_{\star}(x)$ is continuous and continuously differentiable on the interval $[0, \frac{1}{2})$. Furthermore, this function is strictly monotonously increasing on $[0, \frac{1}{2})$ and $\lim_{x \uparrow \frac{1}{2}} M_{\star}(x) = +\infty$.*

Proof. Clearly, one needs to check continuity and continuous differentiability of $M_{\star}(x)$ only at the points \varkappa_n , $n = 1, 2, \dots$. Given $n \in \mathbb{N}$, by (5.7) for $x \in [\varkappa_{n-1}, \varkappa_n)$ we have

$$M_{\star}(x) = \frac{n-1}{2} \arcsin\left(\frac{4\pi}{\pi^2 + 4}\right) + \frac{1}{2} \arcsin\left(\frac{\pi(x - \varkappa_{n-1})}{1 - 2\varkappa_{n-1}}\right), \quad x \in [\varkappa_{n-1}, \varkappa_n). \quad (5.8)$$

Note that (5.1) yields

$$\begin{aligned} \varkappa_n - \varkappa_{n-1} &= \frac{4}{\pi^2 + 4} + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_{n-1} - \varkappa_{n-1} \\ &= \frac{4}{\pi^2 + 4} (1 - 2\varkappa_{n-1}), \quad \text{for all } n \in \mathbb{N}. \end{aligned} \quad (5.9)$$

By (5.9) one observes that

$$\frac{x - \varkappa_{n-1}}{1 - 2\varkappa_{n-1}} \xrightarrow{x \rightarrow \varkappa_n} \frac{\varkappa_n - \varkappa_{n-1}}{1 - 2\varkappa_{n-1}} = \frac{4}{\pi^2 + 4} \quad (5.10)$$

and then from (5.8) it follows that

$$\lim_{x \uparrow \varkappa_n} M_*(x) = \frac{n}{2} \arcsin \left(\frac{4\pi}{\pi^2 + 4} \right). \quad (5.11)$$

Meanwhile, by its definition (5.7) on the interval $x \in [\varkappa_n, \varkappa_{n+1})$, the function $M_*(x)$ is right-continuous at $x = \varkappa_n$ and

$$\frac{n}{2} \arcsin \left(\frac{4\pi}{\pi^2 + 4} \right) = \lim_{x \downarrow \varkappa_n} M_*(x) = M_*(\varkappa_n).$$

Hence, (5.11) yields continuity of $M_*(x)$ at $x = \varkappa_n$.

Using equality (5.9) one more time, one verifies by inspection that for any $n \in \mathbb{N}$ the left and right limiting values

$$\lim_{x \uparrow \varkappa_n} M'_*(x) = \frac{1}{2} \frac{1}{\sqrt{1 - \frac{\pi^2(\varkappa_n - \varkappa_{n-1})^2}{(1 - 2\varkappa_{n-1})^2}}} \frac{\pi}{1 - 2\varkappa_{n-1}} \quad \text{and} \quad \lim_{x \downarrow \varkappa_n} M'_*(x) = \frac{1}{2} \frac{\pi}{1 - 2\varkappa_n}$$

of the derivative $M'_*(x)$ as $x \rightarrow \varkappa_n$ are equal to each other. Hence, for any $n \in \mathbb{N}$ the derivative $M'_*(x)$ is continuous at $x = \varkappa_n$ and then it is continuous on $[0, \frac{1}{2}]$.

Obviously, $M'_*(x) > 0$ for all $x \in (0, \frac{1}{2})$, which means that the function $M_*(x)$ is strictly monotonously increasing on $[0, \frac{1}{2}]$. Then, given any $n \in \mathbb{N}$, from (5.7) it follows that $M_*(x) \geq nC_0$ with $C_0 = \frac{1}{2} \arcsin \left(\frac{4\pi}{\pi^2 + 4} \right) > 0$ whenever $x \geq \varkappa_n$. Taking into account (5.5), this implies that $M_*(x) \rightarrow \infty$ as $x \rightarrow \frac{1}{2}$, completing the proof. \square

Remark 5.2. Since the function $M_*(x)$ is continuous and strictly monotonous on $[0, \frac{1}{2}]$ and $M_*(0) = 0$, $\lim_{x \uparrow \frac{1}{2}} M_*(x) = +\infty$, there is a unique number $c_* \in [0, \frac{1}{2}]$ such that

$$M_*(c_*) = \frac{\pi}{2}. \quad (5.12)$$

An explicit numerical evaluation of

$$C_0 = \frac{1}{2} \arcsin \left(\frac{4\pi}{\pi^2 + 4} \right) \quad (5.13)$$

shows that $C_0 = \frac{\pi}{2} \times 0.360907\dots$. Thus, $2C_0 < \frac{\pi}{2}$ while $3C_0 > \frac{\pi}{2}$. Hence, $c_* \in [\varkappa_2, \varkappa_3]$ and by (5.7), with $n = 2$, equation (5.12) turns into

$$\arcsin \left(\frac{4\pi}{\pi^2 + 4} \right) + \frac{1}{2} \arcsin \left(\frac{\pi(c_* - \varkappa_2)}{1 - 2\varkappa_2} \right) = \frac{\pi}{2}, \quad (5.14)$$

with \varkappa_2 being equal (see (5.2)) to

$$\varkappa_2 = \frac{8\pi^2}{(\pi^2 + 4)^2} = 0.410451\dots \quad \left(> \frac{1}{\pi} \right). \quad (5.15)$$

One verifies by inspection that the solution c_* to equation (5.14), and hence to equation (5.12), reads

$$c_* = 16 \frac{\pi^6 - 2\pi^4 + 32\pi^2 - 32}{(\pi^2 + 4)^4} = 0.454169\dots. \quad (5.16)$$

Proposition 5.3. (Optimality of the function M_* .) Let $\{\mu_n\}_{n=0}^\infty \subset [0, \frac{1}{2})$ be an arbitrary monotonously increasing number sequence such that

$$\mu_0 = 0 \quad \text{and} \quad 0 < \frac{\pi(\mu_n - \mu_{n-1})}{1 - 2\mu_{n-1}} \leq 1 \quad \text{for } n \geq 1. \quad (5.17)$$

Assume that $\sup_n \mu_n := \mu_{\sup}$ and introduce the function $F : [0, \mu_{\sup}] \rightarrow \mathbb{R}$ by

$$F(x)|_{[0, \mu_1]} = \frac{1}{2} \arcsin(\pi x), \quad (5.18)$$

$$F(x)|_{[\mu_n, \mu_{n+1}]} = \frac{1}{2} \sum_{j=1}^n \arcsin \left(\frac{\pi(\mu_j - \mu_{j-1})}{1 - 2\mu_{j-1}} \right) + \frac{1}{2} \arcsin \left(\frac{\pi(x - \mu_n)}{1 - 2\mu_n} \right), \quad n \geq 1, \quad (5.19)$$

The function $M_*(x)$ is optimal in the sense that if $\{\mu_n\}_{n=0}^\infty$ does not coincide with the sequence (5.1), then there always exists an open interval $\mathcal{F} \subset (0, \mu_{\sup})$ such that $F(x) > M_*(x)$ for all $x \in \mathcal{F}$.

Proof. First, we remark that if one chooses $\mu_n = \varkappa_n$, $n = 0, 1, 2, \dots$, where $\{\varkappa_n\}_{n=0}^\infty$ is the sequence (5.1), then F coincides with M_* . If $\{\mu_n\}_{n=0}^\infty \neq \{\varkappa_n\}_{n=0}^\infty$ then there is $m \in \mathbb{N}$ such that $\mu_n = \varkappa_n$ for all $n < m$ and $\mu_m \neq \varkappa_m$. Since, $\mu_{m-1} = \varkappa_{m-1}$, there are two options: either

$$\varkappa_{m-1} < \mu_m < \min\{\varkappa_m, \mu_{m+1}\} \quad (5.20)$$

or

$$\varkappa_m < \mu_m \quad (\text{and } \mu_m < \mu_{m+1}). \quad (5.21)$$

By (5.7) and (5.18), (5.19) in the case (5.20) equality $M_*(x) = F(x)$ holds for all $x \in [0, \mu_m]$. For $x \in (\mu_m, \min\{\varkappa_m, \mu_{m+1}\})$ we have

$$\begin{aligned} M_*(x) &= (m-1)C_0 + \frac{1}{2} \arcsin \left(\frac{\pi(x - \varkappa_{m-1})}{1 - 2\varkappa_{m-1}} \right), \\ F(x) &= (m-1)C_0 + \frac{1}{2} \arcsin \left(\frac{\pi(\mu_m - \varkappa_{m-1})}{1 - 2\varkappa_{m-1}} \right) + \frac{1}{2} \arcsin \left(\frac{\pi(x - \mu_m)}{1 - 2\mu_m} \right), \end{aligned}$$

where C_0 is given by (5.13). Having explicitly computed the derivatives of $M_*(x)$ and $F(x)$ for $x \in (\mu_1, \min\{\varkappa_m, \mu_{m+1}\})$, one obtains that $F'(x) > M'_*(x)$ whenever $\mu_m < x < \xi_m$, where

$$\xi_m = \min \left\{ \mu_{m+1}, \frac{1}{2\pi^2} [4 + (\pi^2 - 4)(\varkappa_{m-1} + \mu_m)] \right\}.$$

Notice that $\xi_m > \mu_m$ since $\mu_{m+1} > \mu_m$ and

$$\begin{aligned} \frac{1}{2\pi^2} [4 + (\pi^2 - 4)(\varkappa_{m-1} + \mu_m)] - \mu_m &= \frac{\pi^2 + 4}{2\pi^2} \left(\frac{4}{\pi^2 + 4} + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_{m-1} - \mu_m \right) \\ &= \frac{\pi^2 + 4}{2\pi^2} (\varkappa_m - \mu_m) \\ &> 0 \end{aligned}$$

(see (5.1) and (5.20)). Observing that $M_*(\mu_m) = F(\mu_m)$, one concludes that $F(x) > M_*(x)$ at least for all x from the open interval $\mathcal{F} = (\mu_m, \xi_m)$.

If (5.21) holds then $M_*(x) = F(x)$ for $x \in [0, \varkappa_m]$. At the same time, for

$$\varkappa_m < x < \min\{\varkappa_{m+1}, \mu_m\} \quad (5.22)$$

we have

$$M_*(x) = (m-1)C_0 + \frac{1}{2} \arcsin \left(\frac{\pi(\varkappa_m - \varkappa_{m-1})}{1-2\varkappa_{m-1}} \right) + \frac{1}{2} \arcsin \left(\frac{\pi(x - \varkappa_m)}{1-2\varkappa_m} \right), \quad (5.23)$$

$$F(x) = (m-1)C_0 + \frac{1}{2} \arcsin \left(\frac{\pi(x - \varkappa_{m-1})}{1-2\varkappa_{m-1}} \right). \quad (5.24)$$

One verifies by inspection that under condition (5.22) the requirement $F'(x) > M'_*(x)$ is equivalent to

$$\begin{aligned} x &> \frac{1}{2\pi^2} [4 + (\pi^2 - 4)(\varkappa_{m-1} + \varkappa_m)] \\ &= \frac{\pi^2 + 4}{2\pi^2} \left(\frac{4}{\pi^2 + 4} + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_{m-1} + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_m \right) \\ &= \frac{\pi^2 + 4}{2\pi^2} \left(\varkappa_m + \frac{\pi^2 - 4}{\pi^2 + 4} \varkappa_m \right) \\ &= \varkappa_m, \end{aligned}$$

by taking into account relations (5.1) at the second step. That is, (5.22) implies $F'(x) > M'_*(x)$. From $M_*(\varkappa_m) = F(\varkappa_m)$ it then follows that $F(x) > M_*(x)$ at least for all x from the open interval $\mathcal{F} = (\varkappa_m, \min\{\varkappa_{m+1}, \mu_m\})$. The proof is complete. \square

Finally, we turn to the main result of this work.

Theorem 5.4. *Given a (possibly unbounded) self-adjoint operator A on the Hilbert space \mathfrak{H} , assume that a Borel set $\sigma \subset \mathbb{R}$ is an isolated component of the spectrum of A , i.e. $\sigma \subset \text{spec}(A)$ and*

$$\text{dist}(\sigma, \Sigma) = d > 0,$$

where $\Sigma = \text{spec}(A) \setminus \sigma$. Let V be a bounded self-adjoint operator on \mathfrak{H} such that

$$\|V\| < d/2 \quad (5.25)$$

and let $L = A + V$ with $\text{Dom}(L) = \text{Dom}(A)$. Then the maximal angle $\theta(\mathfrak{A}, \mathfrak{L})$ between the spectral subspaces $\mathfrak{A} = \text{Ran}(E_A(\sigma))$ and $\mathfrak{L} = \text{Ran}(E_L(\omega))$ of A and L associated with their respective spectral subsets σ and $\omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\sigma)$ satisfies the bound

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_*(\frac{\|V\|}{d}), \quad (5.26)$$

where the estimating function $M_*(x)$, $x \in [0, \frac{1}{2}]$, is defined by (5.7). In particular, if

$$\|V\| < c_* d, \quad (5.27)$$

where c_* is given by (5.16), then the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case, i.e. $\theta(\mathfrak{A}, \mathfrak{L}) < \frac{\pi}{2}$.

Proof. Throughout the proof we assume that $\|V\| \neq 0$ and set

$$x = \frac{\|V\|}{d}. \quad (5.28)$$

The assumption (5.25) implies $x < \frac{1}{2}$. Hence, there is a number $n \in \mathbb{N} \cup \{0\}$ such that $x \in [\varkappa_n, \varkappa_{n+1})$ with \varkappa_n and \varkappa_{n+1} the consecutive elements of the sequence (5.1).

For $n = 0$ the bound (5.26) holds by Remark 4.4 since in this case $\frac{\|V\|}{d} < \frac{4}{\pi^2 + 4} < c_{\pi/4}$ and $M_*(x) = \frac{1}{2} \arcsin(\pi x)$ (see (4.18), (5.1), and (5.7)).

In the case where $n \geq 1$ we introduce the operators

$$V_j = \varkappa_j \frac{d}{\|V\|} V \quad \text{and} \quad L_j = A + V_j, \quad \text{Dom}(L_j) = \text{Dom}(A), \quad j = 0, 1, \dots, n,$$

where \varkappa_j are elements of the sequence (5.1). Since $\varkappa_j < \varkappa_n$ for $j < n$ and $\varkappa_n \leq x$, from (5.28) it follows that

$$\|V_j\| = \frac{\varkappa_j}{x} \|V\| \leq \|V\| < \frac{d}{2}, \quad j = 0, 1, \dots, n.$$

Therefore, the spectrum of the (self-adjoint) operator L_j consists of the two disjoint components

$$\omega_j = \text{spec}(L_j) \cap \mathcal{O}_{\|V_j\|}(\sigma) \quad \text{and} \quad \Omega_j = \text{spec}(L_j) \cap \mathcal{O}_{\|V_j\|}(\Sigma), \quad j = 0, 1, \dots, n.$$

Moreover,

$$\delta_j := \text{dist}(\omega_j, \Omega_j) \geq d - 2\|V_j\| = d(1 - 2\varkappa_j), \quad j = 0, 1, \dots, n. \quad (5.29)$$

By \mathfrak{L}_j we will denote the spectral subspace of L_j associated with its spectral component ω_j , i.e. $\mathfrak{L}_j = \text{Ran}(\mathbb{E}_{L_j}(\omega_j))$. Notice that $L_0 = A$, $\omega_0 = \sigma$, and $\mathfrak{L}_0 = \mathfrak{A}$.

For $0 \leq j \leq n-1$ the operator L_{j+1} may be viewed as a perturbation of the operator L_j , namely

$$L_{j+1} = L_j + W_j, \quad j = 0, 1, \dots, n-1,$$

where

$$W_j := V_{j+1} - V_j = (\varkappa_{j+1} - \varkappa_j) \frac{d}{\|V\|} V.$$

Similarly, we write

$$L = L_n + W, \quad \text{with} \quad W := V - V_n = (x - \varkappa_n) \frac{d}{\|V\|} V.$$

One easily verifies that

$$\omega_{j+1} = \text{spec}(L_{j+1}) \cap \mathcal{O}_{\|W_j\|}(\omega_j), \quad j = 0, 1, \dots, n-1, \quad (5.30)$$

$$\omega = \text{spec}(L) \cap \mathcal{O}_{\|W\|}(\omega_n). \quad (5.31)$$

By taking into account first (5.29) and then (5.9), one observes that

$$\frac{\|W_j\|}{\delta_j} = \frac{(\varkappa_{j+1} - \varkappa_j)d}{\delta_j} \leq \frac{\varkappa_{j+1} - \varkappa_j}{1 - 2\varkappa_j} = \frac{4}{\pi^2 + 4}, \quad j = 0, 1, \dots, n-1, \quad (5.32)$$

and

$$\frac{\|W\|}{\delta_n} = \frac{(x - \varkappa_n)d}{\delta_n} \leq \frac{x - \varkappa_n}{1 - 2\varkappa_n} \quad \left(< \frac{\varkappa_{n+1} - \varkappa_n}{1 - 2\varkappa_n} = \frac{4}{\pi^2 + 4} \right). \quad (5.33)$$

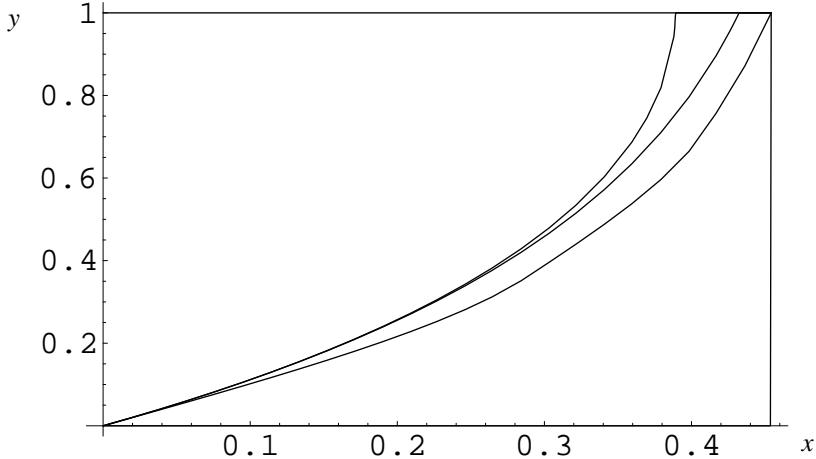


FIGURE 1. Graphs of the functions $\frac{2}{\pi}M_{\text{KMM}}(x)$, $\frac{2}{\pi}M_{\text{MS}}(x)$, and $\frac{2}{\pi}M_*(x)$ while their values do not exceed 1. The upper curve depicts the graph of $\frac{2}{\pi}M_{\text{KMM}}(x)$ for $x \leq c_{\text{KMM}}$, the intermediate curve represents the graph of $\frac{2}{\pi}M_{\text{MS}}(x)$ for $x \leq c_{\text{MS}}$, and the lower curve is the graph of $\frac{2}{\pi}M_*(x)$ for $x \leq c_*$.

Recall that $\frac{4}{\pi^2+4} < c_{\pi/4}$ (see (3.29) and (4.18)). Thus, by (5.30)–(5.33) Remark 4.4 applies to any of the pairs $(\mathfrak{L}_j, \mathfrak{L}_{j+1})$, $j = 0, 1, \dots, n-1$, and $(\mathfrak{L}_n, \mathfrak{L})$, which means that

$$\theta(\mathfrak{L}_j, \mathfrak{L}_{j+1}) \leq \frac{1}{2} \arcsin \left(\frac{\pi \|W_j\|}{\delta_j} \right) \leq \frac{1}{2} \arcsin \left(\frac{4\pi}{\pi^2+4} \right), \quad j = 0, 1, \dots, n-1, \quad (5.34)$$

$$\theta(\mathfrak{L}_n, \mathfrak{L}) \leq \frac{1}{2} \arcsin \left(\frac{\pi \|W\|}{\delta_n} \right) \leq \frac{1}{2} \arcsin \left(\frac{\pi(x - \varkappa_n)}{1 - 2\varkappa_n} \right). \quad (5.35)$$

Meanwhile, by using the triangle inequality for maximal angles between subspaces (see Lemma 2.15) one obtains, step by step,

$$\begin{aligned} \theta(\mathfrak{L}_0, \mathfrak{L}) &\leq \theta(\mathfrak{L}_0, \mathfrak{L}_1) + \theta(\mathfrak{L}_1, \mathfrak{L}) && (\text{if } n \geq 1) \\ &\leq \theta(\mathfrak{L}_0, \mathfrak{L}_1) + \theta(\mathfrak{L}_1, \mathfrak{L}_2) + \theta(\mathfrak{L}_2, \mathfrak{L}) && (\text{if } n \geq 2) \\ &\leq \dots && \dots \\ &\leq \sum_{j=0}^{n-1} \theta(\mathfrak{L}_j, \mathfrak{L}_{j+1}) + \theta(\mathfrak{L}_n, \mathfrak{L}) && (\text{if } n \geq 1). \end{aligned} \quad (5.36)$$

Combining (5.36) with (5.34) and (5.35) results just in the bound (5.26), taking into account equality $\mathfrak{L}_0 = \mathfrak{A}$ and the definitions (5.28) of x and (5.7) of $M_*(x)$. Finally, by Proposition 5.1 and Remark 5.2 one concludes that under condition (5.27) the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case. This completes the proof. \square

Remark 5.5. Recall that the previously known estimating functions for $\theta(\mathfrak{A}, \mathfrak{L})$ are those of references [16] and [19], namely the functions $M_{\text{KMM}}\left(\frac{\|V\|}{d}\right)$ (see Remark 3.8) and $M_{\text{MS}}\left(\frac{\|V\|}{d}\right)$ (see Remark 3.6). One verifies by inspection that the derivatives $M'_{\text{KMM}}(x)$, $M'_{\text{MS}}(x)$, and $M'_*(x)$ of the estimating functions $M_{\text{KMM}}(x)$, $M_{\text{MS}}(x)$, and $M_*(x)$ possess the following properties

$$M'_{\text{MS}}(x) < M'_{\text{KMM}}(x) \quad \text{for all } x \in (0, c_{\text{KMM}}), \quad (5.37)$$

$$M'_*(x) < M'_{\text{MS}}(x) \quad \text{for all } x \in [0, \frac{1}{2}) \setminus \{\varkappa_n\}_{n=0}^\infty, \quad (5.38)$$

$$M'_*(\varkappa_n) = M'_{\text{MS}}(\varkappa_n), \quad n = 0, 1, 2, \dots, \quad (5.39)$$

where c_{KMM} is given by (1.6) and $\{\varkappa_n\}_{n=0}^\infty$ is the sequence (5.1). Since

$$M_{\text{KMM}}(0) = M_{\text{MS}}(0) = M_*(0) = 0,$$

from (5.37)–(5.39) it follows that

$$M_*(x) < M_{\text{MS}}(x) < M_{\text{KMM}}(x) \quad \text{for all } x \in (0, c_{\text{KMM}}]$$

and

$$M_*(x) < M_{\text{MS}}(x) \quad \text{for all } x \in [c_{\text{KMM}}, \frac{1}{2}).$$

Thus, the bound (5.26) is stronger than both the previously known bounds [16, 19] for $\theta(\mathfrak{A}, \mathfrak{L})$, in particular it is stronger than the best of them, the bound (3.25), established in [19].

For convenience of the reader, the graphs of the estimating functions $M_*(x)$, $M_{\text{MS}}(x)$, and $M_{\text{KMM}}(x)$, all the three divided by $\pi/2$, are plotted in Fig. 1. Plotting of the function $\frac{2}{\pi} M_{\text{KMM}}(x)$ is naturally restricted to its domain $[0, c_{\text{KMM}}]$. The functions $M_*(x)$ and $M_{\text{MS}}(x)$ are plotted respectively for $x \in [0, c_*]$ and $x \in [0, c_{\text{MS}}]$ where c_* is given by (5.16) and c_{MS} by (1.7).

We conclude this section with an a posteriori result that is an immediate corollary to Theorem 5.4.

Theorem 5.6. *Assume that A and V are self-adjoint operators on the Hilbert space \mathfrak{H} . Let $V \in \mathcal{B}(\mathfrak{H})$ and $L = A + V$ with $\text{Dom}(L) = \text{Dom}(A)$. Assume, in addition, that ω is an isolated component of the spectrum of L , i.e. $\text{dist}(\omega, \Omega) = \delta > 0$, where $\Omega = \text{spec}(L) \setminus \omega$, and suppose that $\|V\| < \delta/2$. Then the maximal angle $\theta(\mathfrak{A}, \mathfrak{L})$ between the spectral subspaces $\mathfrak{A} = \text{Ran}(\mathsf{E}_A(\sigma))$ and $\mathfrak{L} = \text{Ran}(\mathsf{E}_L(\omega))$ of A and L associated with their respective spectral components $\sigma = \text{spec}(A) \cap \mathcal{O}_{\|V\|}(\omega)$ and ω satisfies the bound*

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_*(\frac{\|V\|}{\delta}) \quad (5.40)$$

with M_* given by (5.7). In particular, if $\|V\| < c_* \delta$ where c_* is given by (5.16), the subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case.

Proof. Do exactly the same step as we did in the proof of Corollary 4.3: Represent A as $A = L + W$ with $W = -V$. Then the assertion follows from Theorem 5.4. \square

Remark 5.7. As usually, let $\Sigma = \text{spec}(A) \setminus \sigma$ and $d = \text{dist}(\sigma, \Sigma)$. Suppose that both the ‘a priori’ and ‘a posteriori’ distances d and δ are known. Then, depending on which of the distances d and δ is larger, one may choose among the bounds (5.26) and (5.40) the stronger one:

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_* \left(\frac{\|V\|}{\max\{d, \delta\}} \right).$$

6. Quantum harmonic oscillator under a bounded perturbation

In this section we apply the results of the previous section to the N -dimensional isotropic quantum harmonic oscillator under a bounded self-adjoint perturbation.

Let $\mathfrak{H} = L_2(\mathbb{R}^N)$ for some $N \in \mathbb{N}$. Under the assumption that the units are chosen such that the reduced Planck constant, mass of the particle, and the angular frequency are all equal to one, the Hamiltonian of the isotropic quantum harmonic oscillator is given by

$$(Af)(x) = -\frac{1}{2}\Delta f(x) + \frac{1}{2}|x|^2 f(x), \\ \text{Dom}(A) = \left\{ f \in W_2^2(\mathbb{R}^N) \mid \int_{\mathbb{R}^N} dx |x|^4 |f(x)|^2 < \infty \right\}, \quad (6.1)$$

where Δ is the Laplacian and $W_2^2(\mathbb{R}^N)$ denotes the Sobolev space of $L_2(\mathbb{R}^N)$ -functions that have their second partial derivatives in $L_2(\mathbb{R}^N)$.

It is well known that the Hamiltonian A is a self-adjoint operator in $L_2(\mathbb{R}^N)$. Its spectrum consists of eigenvalues of the form

$$\lambda_n = n + N/2, \quad n = 0, 1, 2, \dots, \quad (6.2)$$

whose multiplicities m_n are given by the binomial coefficients (see, e.g., [18] and references therein)

$$m_n = \binom{N+n-1}{n}, \quad n = 0, 1, 2, \dots \quad (6.3)$$

For n even, the corresponding eigenfunctions $f(x)$ are symmetric with respect to space reflection $x \mapsto -x$ (i.e. $f(-x) = f(x)$). For n odd, the eigenfunctions are anti-symmetric (i.e. $f(-x) = -f(x)$). Thus, if one partitions the spectrum $\text{spec}(A) = \sigma \cup \Sigma$ into the two parts

$$\sigma = \{n + N/2 \mid n = 0, 2, 4, \dots\} \quad \text{and} \quad \Sigma = \{n + N/2 \mid n = 1, 3, 5, \dots\},$$

then the complementary subspaces

$$\mathfrak{A} = L_{2,\text{even}}(\mathbb{R}^N), \quad \mathfrak{A}^\perp = L_{2,\text{odd}}(\mathbb{R}^N) \quad (6.4)$$

of symmetric and anti-symmetric functions are the spectral subspaces of A corresponding to the spectral components σ and Σ , respectively. Clearly,

$$d = \text{dist}(\sigma, \Sigma) = 1.$$

Let V be an arbitrary bounded self-adjoint operator on $L_2(\mathbb{R}^N)$ such that

$$\|V\| < 1/2. \quad (6.5)$$

The perturbed oscillator Hamiltonian $L = A + V$, $\text{Dom}(L) = \text{Dom}(A)$, is self-adjoint and its spectrum remains discrete. Moreover, the closed $\|V\|$ -neighborhood $\mathcal{O}_{\|V\|}(\lambda_n)$ of the eigenvalue (6.2) of A contains exactly m_n eigenvalues $\lambda'_{n,k}$, $k = 1, 2, \dots, m_n$, of L , counted with multiplicities, where m_n is given by (6.3) (see, e.g., [13, Section V.4.3]).

Further, assume that the following stronger condition holds:

$$\|V\| < c_*, \quad (6.6)$$

where c_* is given by (5.16). Let \mathfrak{L} be the spectral subspace of the perturbed Hamiltonian L associated with the spectral subset $\omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\sigma)$. Theorem 5.4 ensures that under condition (6.6) the unperturbed and perturbed spectral subspaces \mathfrak{A} and \mathfrak{L} are in the acute-angle case. Moreover, the maximal angle $\theta(\mathfrak{A}, \mathfrak{L})$ between these subspaces satisfies the bound

$$\theta(\mathfrak{A}, \mathfrak{L}) \leq M_*(\|V\|), \quad (6.7)$$

where M_* stands for the function given by (5.7).

Obviously, under condition (6.6) the orthogonal complement \mathfrak{L}^\perp is the spectral subspace of L associated with the spectral set $\Omega = \text{spec}(L) \cap \mathcal{O}_{\|V\|}(\Sigma)$. By Remark 2.4, $\theta(\mathfrak{A}^\perp, \mathfrak{L}^\perp) = \theta(\mathfrak{A}, \mathfrak{L})$. Hence the maximal angle between the subspaces \mathfrak{A}^\perp and \mathfrak{L}^\perp satisfies the same bound (6.7), i.e. $\theta(\mathfrak{A}^\perp, \mathfrak{L}^\perp) \leq M_*(\|V\|)$. Surely, this can also be seen directly from Theorem 5.4.

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